PLS Mean Centering

This example shows how to compute Partial Least Squares (PLS) with mean centering.

Supporting Information

A Practical Guide to Chemometric Analysis of Optical Spectroscopic Data

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Partial Least Squares (PLS) with Mean Centering

Partial least squares usually uses mean-centered data to compute C_{pls} using the weights from the SIMPLS algorithm with r latent variables.

```
X = A_train;
Y = C_train;

X0 = X - mean(X,1);
Y0 = Y - mean(Y,1);
[X_loadings, Y_loadings, X_scores, Y_scores, Weights] = pnnl_simpls(X0, Y0, r);

B_pls = Weights * Y_loadings';

C_pls = (A_unknown - mean(A_train,1)) * B_pls + mean(C_train,1);
```

Partial Least Squares (PLS) without Mean Centering

The following is PLS without mean centering.

```
X = A_train;
Y = C_train;

[X_loadings,Y_loadings,X_scores,Y_scores,Weights] = pnnl_simpls(X,Y,r);
```

```
B_pls = Weights * Y_loadings';

C_pls = A_unknown * B_pls;
```

Combined algorithm

To make it easier to run with the rest of the tools in the PNNL toolbox, we combined mean-centered and non-mean-centered into one function with `meanCentered` as an optional argument. When `meanCentered` is not used as an input, then the default is to compute without mean-centered data.

```
function [C_pls, B_pls] = pnnl_pls(A_train, C_train, A_unknown, r, meanCentered)
     if nargin < 5
        meanCentered = false;
    end

    X = A_train;
    Y = C_train;
    if meanCentered
        X0 = X - mean(X,1);
        Y0 = Y - mean(Y,1);
    else
        X0 = X;
        Y0 = Y;
    end

    [X_loadings,Y_loadings,X_scores,Y_scores,Weights] = pnnl_simpls(X0,Y0,r); %#ok<ASGLU>

    B_pls = Weights * Y_loadings';

    if meanCentered
        C_pls = (A_unknown - mean(A_train,1)) * B_pls + mean(C_train,1);
    else
        C_pls = A_unknown * B_pls;
    end
end
```

Napalm Data

Load the included napalm data to run the PLS algorithms.

```
clearvars
load pnnl_napalm_data
whos
```

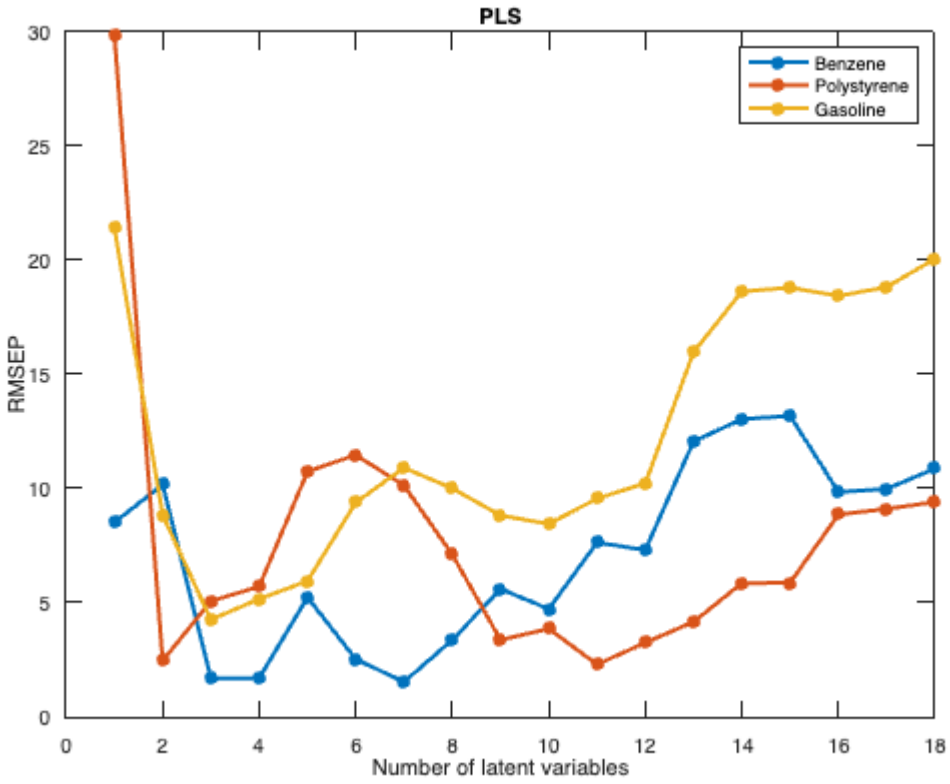
```
  Name                  Size              Bytes  Class     Attributes

  A_train              20x1713           274080  double
  A_unknown            12x1713           164448  double
  C_train              20x3                 480  double
  C_validation         12x3                 288  double
  ConcentrationUnits    1x4                   8  char
  ConstituentNames      1x3                 364  cell
  WavenumberLabel       1x20                 40  char
```

```
Wavenumbers             1x1713             13704  double
ans                     1x1                    8  double
```

Optimal number of latent variables for PLS with mean centering

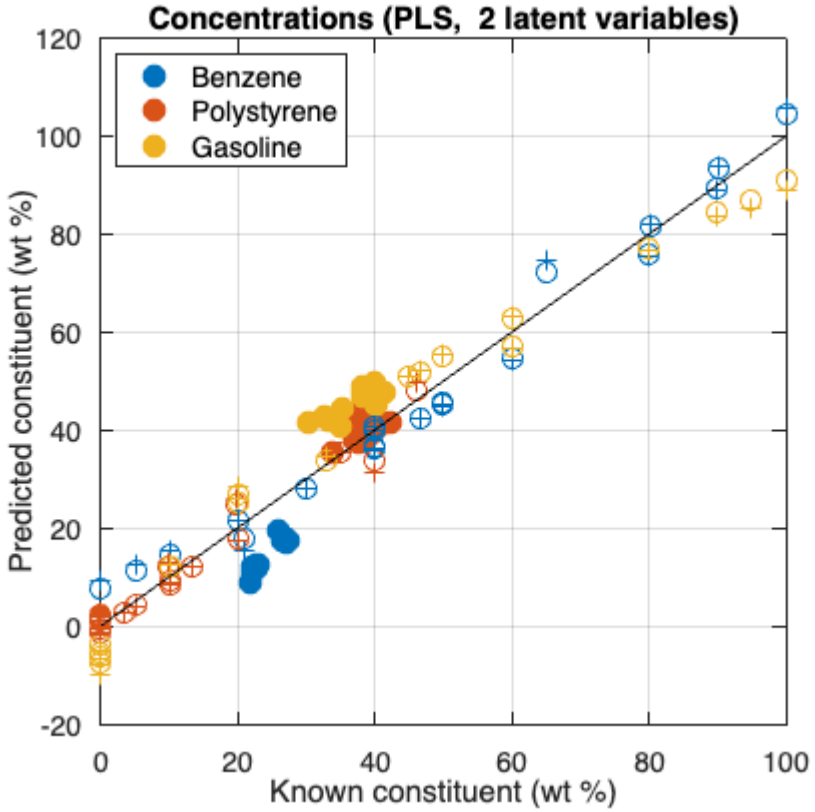
Compute PLS with mean centering for 1 through 18 latent variables and plot RMSEP for them.

```
nLatentVariables = 1:18;
meanCentered = true;
[C_pls, RMSEP_pls] = pnnl_napalm_pls(nLatentVariables,meanCentered);
plot(nLatentVariables, RMSEP_pls,'.-','LineWidth',2,'MarkerSize',20)
xlabel('Number of latent variables')
ylabel('RMSEP')
title('PLS')
legend(ConstituentNames{:})
```



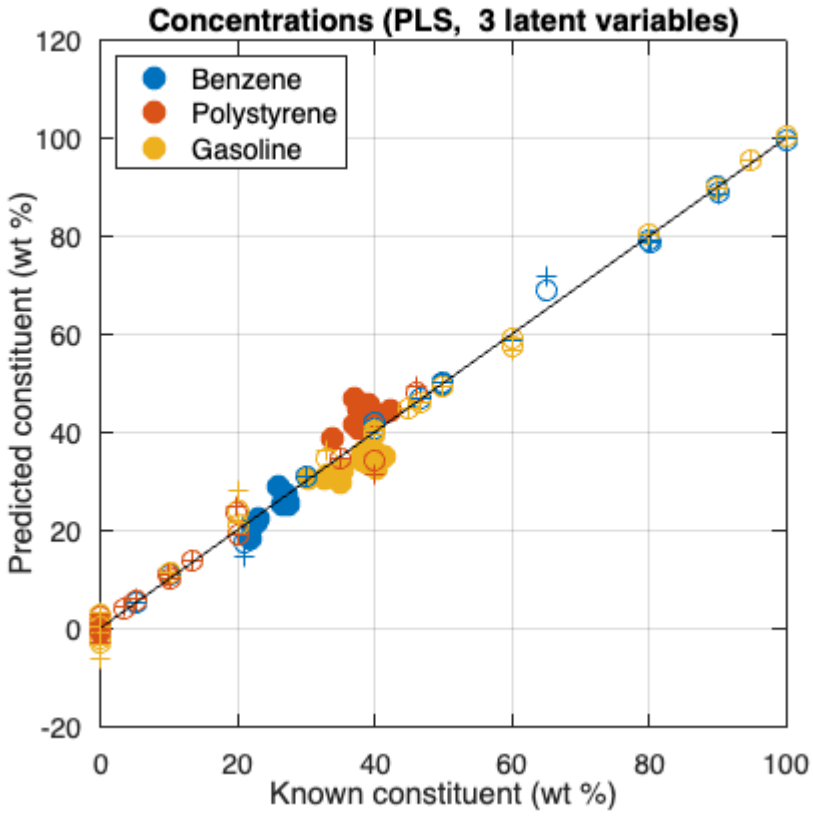
For mean-centered data, it looks like the knee in the curve for polystyrene is 2 latent variables, and 3 for benzene and gasoline. Plot them to see what they look like.

```
nLatentVariables = [2,3];
pnnl_napalm_pls(nLatentVariables,meanCentered);
```



Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

PLS, 2 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	4.1479	2.296	5.5014
RMSECV	5.0229	2.924	6.5258
RMSEP	10.164	2.4566	8.8266

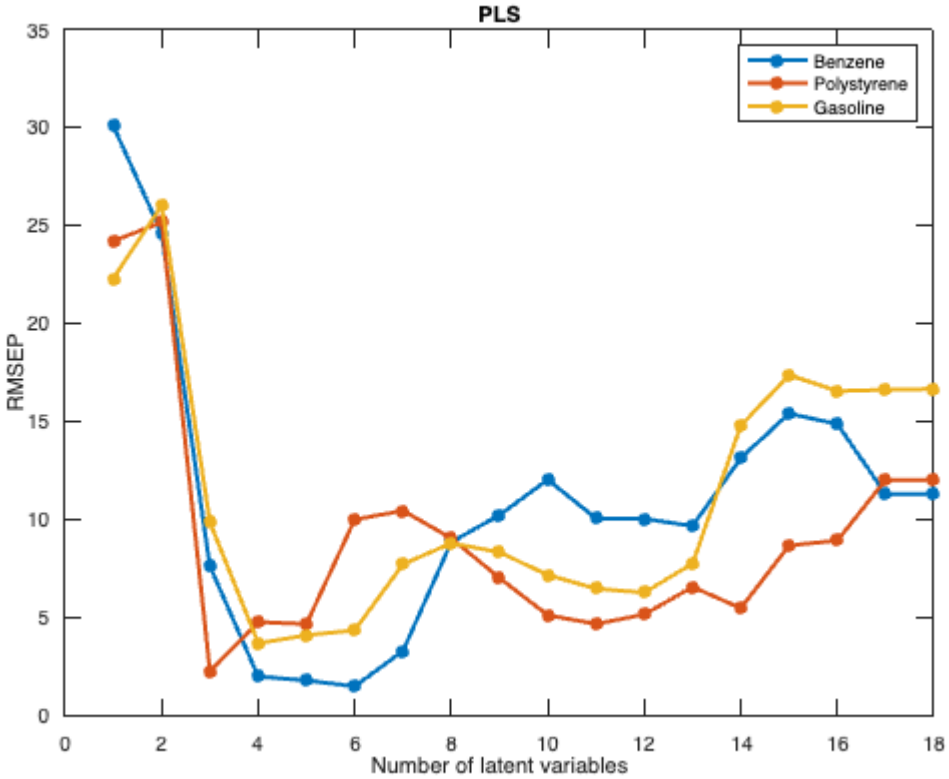



```
Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.
------------------------------------------------------------------------
  PLS,  3 latent variables       Benzene    Polystyrene      Gasoline
                    RMSEC        1.3968         1.8465        1.5789
                   RMSECV        2.2406         2.6176        2.7657
                    RMSEP        1.6799         5.0647        4.2528
------------------------------------------------------------------------
```

Optimal number of latent variables for PLS without mean centering

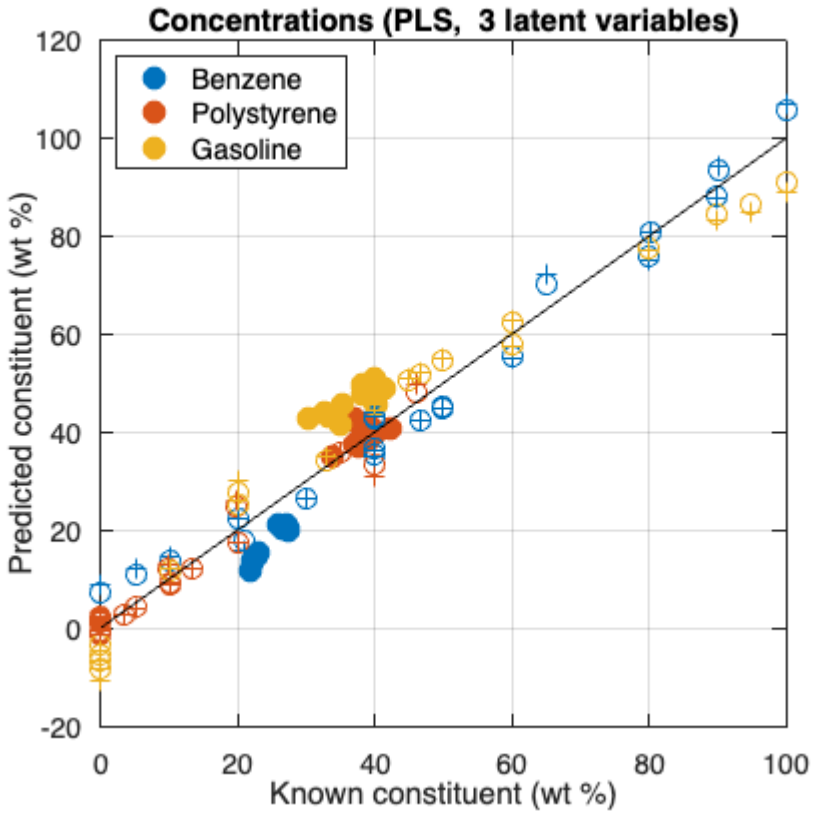
Compute PLS witout mean centering for 1 through 18 latent variables and plot RMSEP for them.

```
nLatentVariables = 1:18;
meanCentered = false;
[C_pls, RMSEP_pls] = pnnl_napalm_pls(nLatentVariables,meanCentered);
plot(nLatentVariables, RMSEP_pls,'.-','LineWidth',2,'MarkerSize',20)
xlabel('Number of latent variables')
ylabel('RMSEP')
title('PLS')
legend(ConstituentNames{:})
```



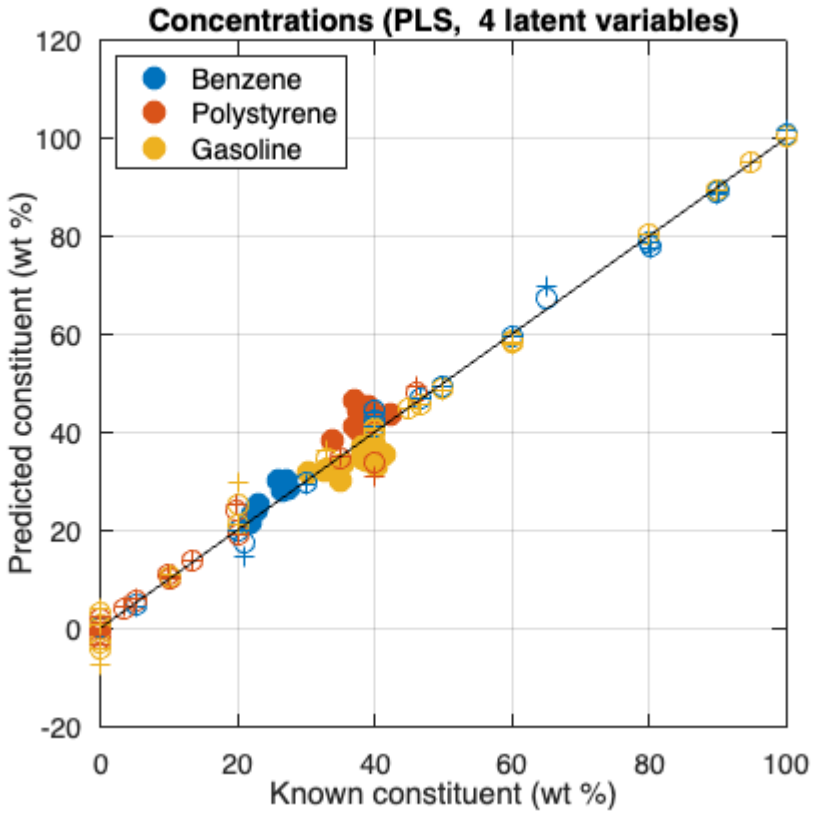
Without mean centering, it looks like the knee in the curve for polystyrene is 3 latent variables, 4 for gasoline, and 6 for benzene. Plot them to see what they look like.

```
nLatentVariables = [3 4 6];
pnnl_napalm_pls(nLatentVariables,meanCentered);
```



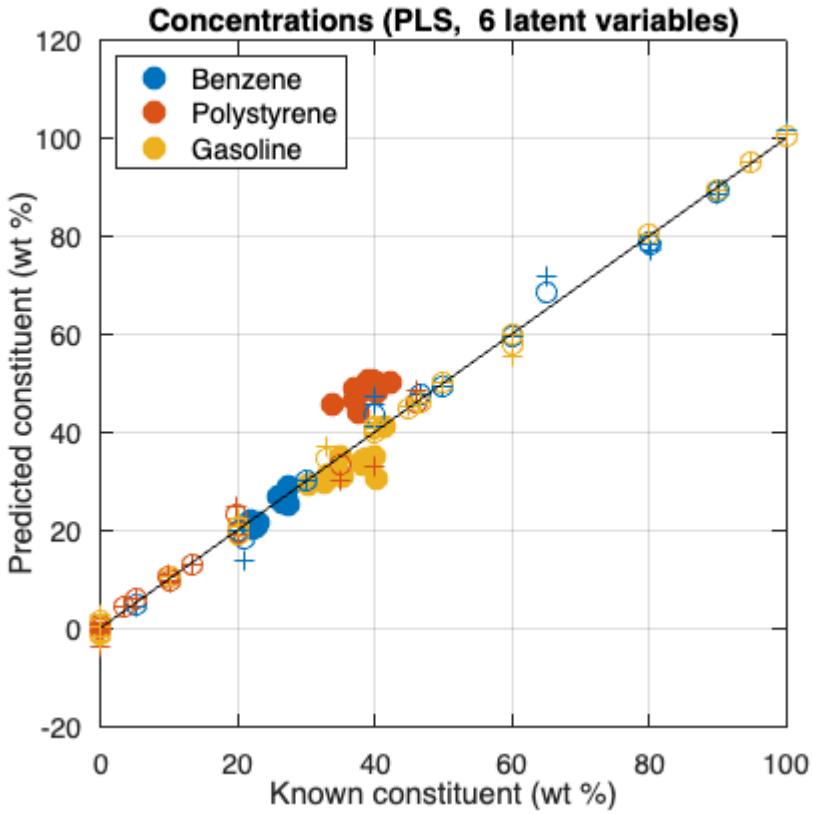
Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

PLS, 3 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	4.1853	2.3592	5.6109
RMSECV	5.0232	2.9897	6.6976
RMSEP	7.5851	2.2404	9.8369



Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

PLS, 4 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	1.6636	1.921	1.9509
RMSECV	2.3112	2.6884	3.2095
RMSEP	1.9599	4.7379	3.6527




```
Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.
-------------------------------------------------------------------------
  PLS,  6 latent variables       Benzene    Polystyrene       Gasoline
                    RMSEC        1.4134        0.99256        0.91242
                   RMSECV        3.1544         2.5526         1.7502
                    RMSEP        1.4567         9.9656         4.3211
-------------------------------------------------------------------------
```

Suppresss editor warnings in this file.

```
%#ok<*ASGLU>
```

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